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Quantized ionic conductance in nanopores¹ MICHAEL ZWOLAK, Los Alamos National Laboratory, JOHAN LAGERQVIST, MASSIMILIANO DI VENTRA, University of California - San Diego — We study ion transport through nanopores via molecular dynamics calculations. Due to the confined geometry and large local field of a single ion, the nanoscale atomic configurations of species influence the ionic conductance. In particular, hydration layers that form around ions in aqueous solution create a series of energy barriers to ion transport. As an ion enters the pore, these hydration layers have to be partially broken due to steric restrictions of the pore. The breaking of the layers proceeds in a highly nonlinear, step-like fashion, giving rise to a strong nonlinear dependence of the electrostatic energy barrier on the pore diameter and therefore also a step-like conductance. We discuss this effect as well as the conditions under which it may be experimentally observed.

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